Stochastic Multiscale Material Modeling

Todd O. Williams, T-3

All materials are heterogeneous at the microstructural length scale. Furthermore, the vast majority of these materials have random microstructures. High explosives (HEs) and continuous fiber composites, shown in Fig. 1, are both examples of such materials that are of interest to Los Alamos National Laboratory (LANL) as well as to U.S. Department of Energy (DOE) and civil applications.

The extremes in the statistical variations of the material microstructures drive important phenomena such as inelastic behavior and failure. The inelastic behavior and failure of such materials has many obvious implications for many types of analysis (for example, safety analyses). The only hope for correctly capturing the effects of these extremes on the local and bulk material behavior is through the use of stochastic analyses.

A new stochastic, multiscale model has been developed for modeling the constitutive behavior of HEs as well as other types of heterogeneous materials [1]. The formulation utilizes localization relations of the form

$$\varepsilon'(a) = A'(a)\bar{\varepsilon} + \int_{b_-}^{b_+} d'(a,b)(\bar{\mu} + \mu'(b))P(b)db$$

where $\varepsilon'(a)$ is the fluctuating strain, $A'(a)$ is the mechanical concentration tensor that describes how the applied bulk (average) strain $\bar{\varepsilon}$ maps into localization effects, $d'(a,b)$ is the transformation concentration tensor that determines how the distribution of transformation strains (eigenstrains) $\mu(b)$ maps into the fluctuating strain field, a and b are both the set of independent variables that describe the configurational possibilities for the material microstructure, b_+ and b_- are the range of b, and $P(b)$ is the probability distribution function (PDF) for the configurational variable.

Using a hierarchical decomposition, the concentration tensors in the different phases in the bulk material are separated into components associated with a phase average fluctuating response (PAFF) and the associated phase zero mean fluctuating response (PZMFF), i.e.,

$$A' = \sum_r A'_r X_r = \sum_r (\hat{A}_r + A''_r) X_r =$$

$$\sum_r \left[c_r^{-1} \int_{a_-}^{a_+} A'(a) X_r(a) P(a) da + A''_r \right] X_r$$

where c_r is the volume fraction of the r^{th} phase and $X_{r(a)}$ is the characteristic function which has a value of 1 in the r^{th} phase and zero otherwise. For a two-phase material, the hierarchical decomposition allows the transformation field concentration tensor $d'(a,b)$ to be completely described in terms of the mechanical concentration tensor $A'(a)$. In this case the statistics required to correctly describe the material behavior are substantially reduced.

Currently the input for the theory is the PDFs for the concentration tensors. The distributions for the concentration tensors can be obtained using direct numerical simulations (DNS), various types of analytical micromechanical models (AMM), or any combination of these techniques. Ongoing collaborations with T-1 (DNS) and T-14 (DNS) at LANL as well as the University of South Carolina (AMM) are being pursued with regard to using different techniques to generate the PDFs for the concentration tensors. Sample distributions for a continuous fiber composite are given in Fig. 2.

Given the distributions for the concentration tensors the proposed theory can be used to predict the range of local and bulk responses of a material, as shown in Fig. 3.

For more information contact Todd Williams at oakhill@lanl.gov.

[1] T.O. Williams, "A General, Stochastic Transformation Field Theory," submitted to *J. Eng. Mech.* (2006) in press.

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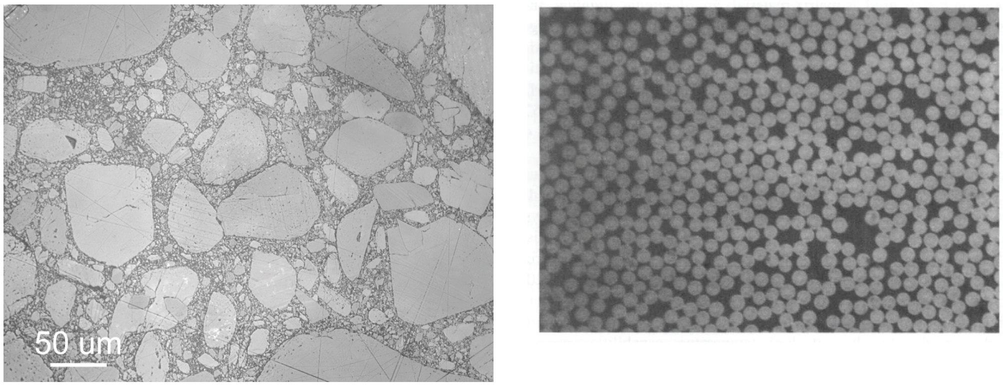

Fig. 1.
Micrographs of a high explosive (left) and a continuous fiber composite (right).

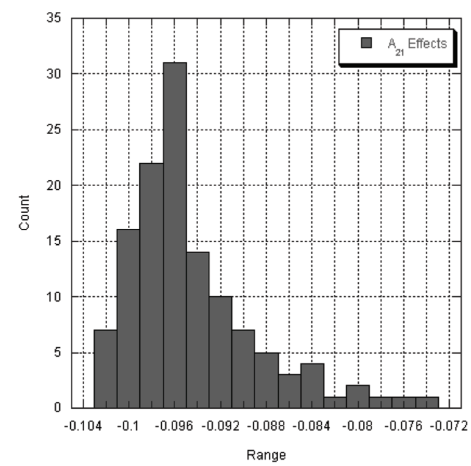

Fig. 2.
The phase average fluctuating response (PAFF) (left) and phase zero mean fluctuating response (PZMFF) (right) distributions for a continuous fiber composite.

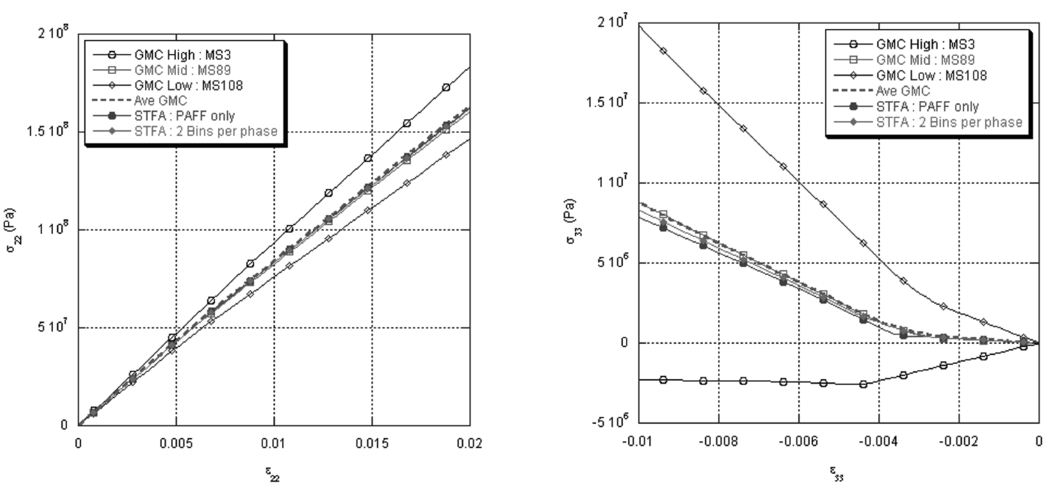

Fig. 3.
The predicted bulk response of a continuous fiber composite subjected to a tri-axial loading state.

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